

# Quantum Disentanglement in Long-range Orders and Spontaneous Symmetry Breaking

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## Abstract

We investigate the nature of quantum entanglement in long-range orders and spontaneous symmetry breaking. It is shown that diminishing of entanglement between the condensate mode and the rest of the system underlies off-diagonal long-range order, which is the hallmark of superconductivity and Bose-Einstein condensation. It is also revealed that disentanglement underlies various cases of long-range order and spontaneous symmetry breaking. In the course of the discussion, we also present some ideas on characterizing entanglement in many-body systems. Especially, it is shown how the connected correlation functions can be used in characterizing entanglements in a pure state.

**Key words:** disentanglement, entanglement, long-range order, spontaneous symmetry breaking

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## 1. Introduction

Long-range order and spontaneous symmetry breaking (SSB) are of great importance in quantum condensed matter physics [1]. Perhaps the most popular examples are ferromagnetism and three-dimensional antiferromagnetism. Off-diagonal long-range order (ODLRO) is the hallmark of Bose-Einstein condensation and superconductivity [2, 3], which may also be conveniently described in terms of SSB of gauge symmetry. SSB of gauge symmetry is also important in high energy physics.

In this Letter, we address the following question: what is the feature of quantum entanglement in the quantum states underlying the phenomena of long-range order and spontaneous symmetry breaking. As a special kind of correlation, quantum entanglement refers to the situation that the quantum state of a composite system is not a direct product of those of the subsystems [4]. It is an essential quantum feature [5, 6]. For many years, this concept has been of central interest in foundations of quantum mechanics. Recently it has been studied in the context of quantum information. As a basic concept in quantum mechanics, it should be useful for, and can be studied in the context of, many-body physics (cf. Refs. [7, 8, 9, 10] and references therein). Here we show that disentanglement, i.e. diminishing of entanglement, underlies long-range orders, including both off-diagonal and “diagonal” long-range orders. Ground state disentanglement in presence of interaction provides a useful insight on SSB and underlies the success of Landau theory of order and phase transition, which is essentially classical. We also explore entanglement characterizations suitable for many-body physics.

## 2. Finite-temperature entanglement

At zero temperature, a closed system is described as a pure state. Hence one can use partial entropy  $S(A)$  of a subsystem  $A$  as the measure of the bi-partite entanglement between  $A$  and its complementary subsystem [11].

At a finite temperature, a reasonable measure is the thermal ensemble average of the entanglements in the Hamiltonian eigenstates. For each Hamiltonian eigenstate  $i$ , as a pure state, one can use partial entropy  $S(A)$  of a subsystem  $A$  as the measure of the bi-partite entanglement between  $A$  and its complementary subsystem. Thus for a thermal ensemble, the bi-partite entanglement is measured by  $\langle S(A) \rangle \equiv \sum_i p_i(T) S_i(A)$ , where  $p_i(T)$  is the statistical distribution at temperature  $T$ ,  $i$  denotes the Hamiltonian eigenstates. The convexity of entropy implies

$$S_{\rho(T)}(A) \geq \langle S(A) \rangle \geq 0, \quad (1)$$

where  $\rho(T) = \sum_i p_i(T) |i\rangle\langle i|$ ,  $S_{\rho(T)}(A)$  is the partial entropy of  $A$  for  $\rho(T)$ . Thus  $S_{\rho(T)}(A)$  is the upper bound of the thermal average entanglement  $\langle S(A) \rangle$ .

We remark that the “mixed-state entanglement measures” studied in quantum information literature, e.g. the so-called concurrence [12], are not suitable for thermal ensembles in statistical physics. In quantum information literature, a “mixed state entanglement” is obtained by considering all possible ensembles mathematically described by the same density matrix. A thermal ensemble, on the other hand, is physically fixed in terms of the Hamiltonian eigenstates. With this physical constraint, it is not physically meaningful to decompose the thermal density matrix in terms of other ensembles. For a density matrix of a subsystem obtained by tracing over the complementary subsystem in a pure state of a

larger system, concurrence may be useful.

### 3. Density matrices and entanglement of identical particles

For a system of  $N$  identical particles, consider the density matrix in Fock space,

$$\langle n'_1 \cdots n'_\infty | \rho | n_1 \cdots n_\infty \rangle,$$

where  $n_k$  or  $n'_k$  represent the occupation number of the single particle state  $k$ . The physical constraints such as particle number conservation and Pauli principle for fermions make many matrix elements vanish.

The reduced density matrix of the occupation-numbers of a set of single particle states  $1, \dots, l$  is

$$\begin{aligned} & \langle n'_1 \cdots n'_l | \rho_l(1 \cdots l) | n_1 \cdots n_l \rangle \\ &= \sum_{n_{l+1} \cdots n_\infty} \langle n'_1 \cdots n'_l, n_{l+1} \cdots n_\infty | \rho | n_1 \cdots n_l, n_{l+1} \cdots n_\infty \rangle. \end{aligned}$$

For a pure state of a fixed number of identical particles, the entanglement, in a given single particle basis, means superposition of different Slater determinants/permanents, and can be quantified in terms of occupation-number entanglement [8].

The upper bound of the ensemble average entanglement between the occupation-numbers of single particle states  $1 \cdots l$  and those of other single particle states is thus given by the von Neumann entropy of  $\rho_l(1 \cdots l)$  obtained from  $\rho(T)$ . For example, for one mode  $k$ , the von Neumann entropy of  $\rho_1(k)$  is

$$S(k) = - \sum_{n_k} \langle n_k | \rho_1(k) | n_k \rangle \log \langle n_k | \rho_1(k) | n_k \rangle. \quad (2)$$

For bosons, the summation in (2) is over  $n_k = 0, \dots, N$ ,  $S(k)$  reaches the maximal value  $\log N$  when  $\langle n_k | \rho_1(k) | n_k \rangle$  is the same for all these values of  $n_k$ . For fermions, the summation is over  $n_k = 0, 1$ , and the maximum of  $S(k)$  is  $\log 2$ . For both bosons and fermions,  $S(k)$  reaches the minimum 0 when  $\langle n_k | \rho_1(k) | n_k \rangle$  is 1 for one value of  $n_k$  and is 0 otherwise. In general, the more inhomogeneous the distribution of  $\langle n_k | \rho_1(k) | n_k \rangle$  for different values of  $n_k$ , the smaller  $S(k)$ . Similar feature is exhibited by the von Neumann entropy of the Fock-space reduced density matrix of more than one mode, for the eigenmodes of this reduced density matrix.

In terms of the states of the *particles*, the density matrix in *configuration space* is

$$\langle k'_1 \cdots k'_N | \rho | k_1 \cdots k_N \rangle,$$

while  $i$ -particle reduced density matrix is given by

$$\langle k'_1 \cdots k'_i | \rho^{(i)} | k_1 \cdots k_i \rangle = \text{Tr}(a_{k'_1} \cdots a_{k'_i} \rho a_{k_i}^\dagger \cdots a_{k_1}^\dagger),$$

with  $\text{Tr} \rho^{(i)} = N(N-1) \cdots (N-i+1)$ .

The following equation is a relation between the reduced density matrices in configuration space and the reduced density matrices in Fock space:

$$\begin{aligned} \text{Tr}[\rho(a_k^\dagger a_k)^i] &= \sum_{n_1 \cdots n_\infty} n_k^i \langle n_1 \cdots n_\infty | \rho | n_1 \cdots n_\infty \rangle \\ &= \sum_{n_k=1}^N n_k^i \langle n_k | \rho_1(k) | n_k \rangle, \end{aligned} \quad (3)$$

where  $i = 1, \dots, N$ .

We mention that for many-body systems, the particle reduced density matrices are related to such quantities as density and distribution functions, hence in principle the entanglement is experimentally measurable.

#### 4. ODLRO leads to disentanglement between the condensate mode and the rest of system

First let us consider bosons, for which one obtains from (3),

$$\begin{pmatrix} 1 & 2 & \dots & N \\ 1 & 2^2 & \dots & N^2 \\ \cdot & \cdot & \dots & \cdot \\ 1 & 2^N & \dots & N^N \end{pmatrix} \begin{pmatrix} \langle 1 | \rho_1(k) | 1 \rangle \\ \langle 2 | \rho_1(k) | 2 \rangle \\ \dots \\ \langle N | \rho_1(k) | N \rangle \end{pmatrix} = \begin{pmatrix} Tr(\rho a_k^\dagger a_k) \\ Tr[\rho(a_k^\dagger a_k)^2] \\ \dots \\ Tr[\rho(a_k^\dagger a_k)^N] \end{pmatrix}. \quad (4)$$

Bose-Einstein condensation is characterized by ODLRO in one-particle reduced density matrix  $\rho^{(1)}$ , i.e.  $\langle \mathbf{x}' | \rho^{(1)} | \mathbf{x} \rangle \neq 0$  as  $|\mathbf{x} - \mathbf{x}'| \rightarrow \infty$ , which is equivalent to the existence of an eigenvalue of order  $N$ , i.e

$$\rho^{(1)} = \lambda_0^{(1)} |\lambda_0^{(1)}\rangle \langle \lambda_0^{(1)}| + \sum_{j \neq 0} \lambda_j^{(1)} |\lambda_j^{(1)}\rangle \langle \lambda_j^{(1)}|, \quad (5)$$

where  $\lambda_0^{(1)} = N\alpha$ ,  $\alpha$  is a finite fraction. Hence (5) can also be used as a definition of Bose-Einstein condensation [13].

Let us consider Eq. (4) in the eigen-basis of  $\rho^{(1)}$ , i.e.  $\{|k\rangle\}$  is given by  $\{|\lambda_j^{(1)}\rangle\}$ . Let  $|k_0\rangle \equiv |\lambda_0^{(1)}\rangle$ . For a given set of  $Tr[\rho(a_k^\dagger a_k)^i]$ ,  $i = 1, \dots, N$ , there is a unique set of  $\langle n_k | \rho_1(k) | n_k \rangle$ , where  $n_k = 0, 1, \dots, N$ . For  $k = k_0$ ,  $Tr(\rho a_{k_0}^\dagger a_{k_0}) = N\alpha$ , while  $Tr[\rho(a_{k_0}^\dagger a_{k_0})^i] \approx N^i \alpha^i$  for  $i = 2, \dots, N$ . If  $Tr[\rho(a_{k_0}^\dagger a_{k_0})^i]$  is exactly  $N^i \alpha^i$  and  $N\alpha$  is an integer, e.g. when  $\alpha = 1$ , then  $\langle N\alpha | \rho_1(k_0) | N\alpha \rangle = 1$  while  $\langle n_{k_0} | \rho_1(k_0) | n_{k_0} \rangle = 0$  for  $n_{k_0} \neq N\alpha$ , consequently  $S(k_0) = 0$ . More generally, the values of  $\langle n_{k_0} | \rho_1(k_0) | n_{k_0} \rangle$  corresponding to one or very few values of  $n_{k_0}$  very close to  $N\alpha$  are finite fractions. Since  $\sum_{n_{k_0}} \langle n_{k_0} | \rho_1(k_0) | n_{k_0} \rangle = 1$ , there can be only very few, typically only one, finite fraction.

Thus ODLRO at  $k_0$  generally implies that  $S(k_0)$  is very small. Typically, suppose  $\langle I(N\alpha) | \rho_1(k_0) | I(N\alpha) \rangle$  is a finite fraction  $\gamma$ , where  $I(N\alpha)$  denotes the integer closest to  $N\alpha$ , while  $\langle n_{k_0} | \rho_1(k_0) | n_{k_0} \rangle$  for  $n_{k_0} \neq I(N\alpha)$  is of the order of  $(1 - \gamma)/N$ . Then  $S(k_0) \approx -\gamma \log \gamma$ , which is very small. With  $S(k)$  being the upper bound, the bi-partite entanglement between the occupation-number at  $k_0$  and the rest of the system is thus also very small, approaching 0 when  $\alpha \rightarrow 1$ . We refer to such diminishing of entanglement as disentanglement.

Therefore Bose-Einstein condensation signals disentanglement between the occupation-number of the condensate mode and the rest of the system. Likewise, for a fragment condensation, in which there are more than one condensate mode, disentanglement occurs respectively between each condensate mode and its complementary subsystem.

Now consider fermions. From Eq. (3), one obtains  $Tr[\rho(a_k^\dagger a_k)^i] = \langle 1 | \rho_1(k) | 1 \rangle \leq 1$ , which does not lead to a particular specification on the nature of entanglement between one mode and others. Indeed, there cannot be ODLRO in  $\rho^{(1)}$  [2], thus there is no ODLRO-induced disentanglement between one fermion mode and others (the non-entangled ground state of a fermi liquid [7] is not the concern here). Moreover, one

can evaluate  $\langle n_{k_1} n_{k_2} \rangle$ ,  $\langle (n_{k_1} + 1) n_{k_2} \rangle$ ,  $\langle n_{k_1} (n_{k_2} + 1) \rangle$  and  $\langle (n_{k_1} + 1) (n_{k_2} + 1) \rangle$ , obtaining  $\langle 00 | \rho_2(k_1, k_2) | 00 \rangle = \langle n_{k_1} n_{k_2} \rangle - \langle n_{k_1} \rangle - \langle n_{k_2} \rangle + 1$ ,  $\langle 01 | \rho_2(k_1, k_2) | 01 \rangle = \langle n_{k_2} \rangle - \langle n_{k_1} n_{k_2} \rangle$ ,  $\langle 10 | \rho_2(k_1, k_2) | 10 \rangle = \langle n_{k_1} \rangle - \langle n_{k_1} n_{k_2} \rangle$ ,  $\langle 11 | \rho_2(k_1, k_2) | 11 \rangle = \langle n_{k_1} n_{k_2} \rangle$ . It can be seen that there is no ODLRO-induced disentanglement between the occupation-numbers of two fermion modes and the rest of the system.

However, for both bosons and fermions, there can be ODLRO in the two-particle reduced density matrix, i.e.

$$\rho^{(2)} = \lambda_0^{(2)} |\lambda_0^{(2)}\rangle \langle \lambda_0^{(2)}| + \sum_{j \neq 0} \lambda_j^{(2)} |\lambda_j^{(2)}\rangle \langle \lambda_j^{(2)}|, \quad (6)$$

where  $\lambda_0^{(2)} = N\delta$ ,  $\delta$  is a finite fraction.  $\sum_j \lambda_j^{(2)} = N(N-1)$ . For fermions  $\lambda_0^{(2)} \leq N$ , and ODLRO in  $\rho^{(2)}$  is a characterization of superconductivity [2]. Note the difference between “a two-particle mode” and “two one-particle modes”. The former is a unitary transformation of the latter in the two-particle Hilbert space, and can be written as  $|K\rangle = \sum_{k_1, k_2} U_{K, (k_1, k_2)} |k_1, k_2\rangle$ . The associated creation operator is  $b_K^\dagger = \sum_{k_1, k_2} U_{K, (k_1, k_2)} a_{k_1}^\dagger a_{k_2}^\dagger$ .  $b_K^\dagger b_K$  gives the number of particle pairs in mode  $K$ , with the maximum  $N(N-1)$ . There are overlaps between different pairs in terms of the original particles. One obtains

$$\text{Tr}[\rho(b_K^\dagger b_K)^j] = \sum_{n_K=1}^{N(N-1)} n_K^j \langle n_K | \rho_2(K) | n_K \rangle, \quad (7)$$

with  $j = 1, \dots, N(N-1)$ .

Following an argument similar to the above one for ODLRO in  $\rho^{(1)}$ , one can find that ODLRO in  $\rho^{(2)}$  implies disentanglement between the occupation-number of the two-particle condensate mode  $|\lambda_0^{(2)}\rangle$  and the rest of the system.

In general, for both bosons and fermions, it can be shown that if there is ODLRO in  $\rho^{(i)}$ , there is disentanglement between the occupation-number of the  $i$ -particle condensate mode and others in the eigen-basis of  $\rho^{(i)}$ . For bosons, ODLRO in  $\rho^{(i)}$  implies ODLRO in  $\rho^{(j)}$  with  $j > i$  [2] and thus also disentanglement between the occupation-number of the  $j$ -particle condensate mode and its complementary subsystem.

The disentanglement of the occupation number of the condensate mode from the system is consistent with the well known result, as used in Bogoliubov theory, that the occupation number of the condensate mode is approximately a constant, which implicates that the system is an eigenstate of the occupation number of the condensate mode. This disentanglement also justifies the (classical) two-fluid model of superfluidity.

## 5. Long-range order and spontaneous Symmetry breaking

Disentanglement also underlies “diagonal” long-range orders, e.g. ferromagnetic state  $|\uparrow \dots \uparrow\rangle$  and antiferromagnetic Néel state  $|\uparrow \downarrow \uparrow \dots \uparrow \downarrow\rangle$ , which are product states. They are enforced by energetics and spontaneous symmetry breaking (SSB). Suppose the square of the sum of the spin operators is  $S^2$ , which commutes the Heisenberg Hamiltonian. The lowest energy states of a ferromagnet is the eigenstates with  $S^2 = Ns(Ns+1)$ , where  $N$  is the number of sites,  $s$  is each spin. The lowest energy state of an antiferromagnet is a singlet  $S^2 = 0$ . Because of SSB, the physical ground state of a ferromagnet is a ferromagnetic state in a certain direction, rather than a superposition state of ferromagnetic states in different

directions. The antiferromagnetically ordered state, i.e. a Néel state, is not even an energy eigenstate.

The point of view of disentanglement can provide insights on the nature of SSB. For large  $N$ , a superposition state is a macroscopic superposition, which is highly fragile under perturbations. As a “Schrödinger cat”, it normally reduces to a basis product state. The ferromagnetic state or antiferromagnetic Néel state is favored over other basis states because they correspond to the lowest energy among the basis states. Ferromagnetism and antiferromagnetism represent two different types of SSB [14]. Disentanglement appears to provide a unified insight. Usually SSB is attributed to the near degeneracy between the symmetric states and thus the stability of the symmetry-breaking states. Complementarily, decoherence due to the coupling with the environment is also useful in explaining SSB. More discussions on this aspect will be made elsewhere.

On the other hand, the stabilization of the singlet state in a low dimensional antiferromagnet may be understood as due to higher tunnelling rate between different product basis states, or lower decoherent rate of the singlet state. This point of view may be supported by the fact that both the tunneling rate and the scattering cross section have dimensional dependence (in general, decoherence rate may be proportional to a certain scattering cross section, cf. [15]). Without perturbation, the tunnelling between different ferromagnetic states is zero in any dimension since it is a Hamiltonian eigenstate.

Disentanglement also provides insights on SSB of gauge symmetry, as a description of Bose condensation and superconductivity. For a closed system, this description is an approximation [14]. We think that the excellence of this approximation is not only because of giving the peaked particle number and energy, but also because ODLRO or disentanglement makes it a good approximation to write  $\langle \hat{\psi}^\dagger(\mathbf{x}')\psi(\mathbf{x}) \rangle$  as  $\langle \hat{\psi}^\dagger(\mathbf{x}') \rangle \langle \psi(\mathbf{x}) \rangle$ , where the average is over a particle number non-conserved (“coherent”) state. The difference with the genuine SSB is that it is merely determined by energetics, disentanglement happens without external perturbation or environment-induced decoherence. For an open system, it may be viewed as a genuine SSB [1, 16]. It may be understood as that, like antiferromagnetism, the system disentangles or decoheres into a “coherent state”, which is not the Hamiltonian eigenstate. The reason why the “coherent state” basis is favored may be related to its robustness [17].

With the long-range order, the system is characterized by the order parameter, which is usually given by the average expectation value of the concerned operator, e.g.  $\langle \sum \hat{s}_{iz} \rangle$  for the ferromagnetism or  $\langle \hat{\psi}(\mathbf{x}) \rangle$  for the Bose condensation. With disentanglement, it is directly related to the state of each single particle. In fact, the order parameter of Bose-Einstein condensation can be directly chosen to be the single particle wavefunction [13]. We see that just because the quantum state is, to the zeroth-order approximation, a (disentangled) product of a same single particle state (in the case of Néel state, it is a product of two opposite spin states), it can be described by such an order parameter, upon which the Landau theory is based. The quantum fluctuation over the order parameter, for example, the spin wave in a ferromagnet or the quantum correction in Bose-Einstein condensation, is related to the small nonzero entanglement.

In relativistic quantum field theory, with SSB, the scalar field is in a particular vacuum among the degenerate vacua, rather than a superposition of different vacua. Similar to the condensed matter cases, usually the SSB is assured by the vanishing of the matrix elements between symmetry breaking vacua. We leave for future discussions the subtle details related to the present discussion, for example, whether decoherence due to the coupling with another degree of freedom, say, the gauge field, may be possible, and the nature of entanglement in

the symmetry breaking vacuum.

## 6. Correlation functions and fluctuations

Several quantities are used in characterizing order or fluctuation. The first is correlation function (or staggered correlation function in the case of antiferromagnetism), i.e. the average of products of operators at different sites, e.g.  $\langle \hat{s}_{iz} \hat{s}_{jz} \rangle$ . The second is the connected correlation function, e.g.  $\langle \hat{s}_{iz} \hat{s}_{jz} \rangle_c \equiv \langle \hat{s}_i \hat{s}_j \rangle - \langle \hat{s}_i \rangle \langle \hat{s}_j \rangle$ . The third is the fluctuation amplitude of an operator  $\hat{O}$ , given by  $\langle \hat{O}^2 \rangle - \langle \hat{O} \rangle^2$ .

Long-range order means the nonvanishing of, say,  $\langle \hat{s}_{iz} \hat{s}_{jz} \rangle$  when the distance between  $i$  and  $j$  approaches infinity. It reaches maximum when the state is the ferromagnetic or Néel state. In a generic superposition state, it is small for large distance. It would still be large if the state could be a superposition of different ferromagnetic or antiferromagnetic Néel state, which is, however, excluded by SSB.

Thus long-range order in  $\hat{s}_{iz}$ , as quantified by the correlation function, may signal the disentanglement into the ferromagnetic or antiferromagnetic state in  $z$  direction.

The relation between disentanglement and long-range order can also be exemplified by the two limits of a quantum Ising model in a transverse field,  $H = J \sum \hat{s}_{iz} \hat{s}_{jz} + B \sum \hat{s}_{ix}$ . In the strong interaction limit, as a simple Ising model, there is SSB, long-range order and disentanglement, as discussed above. In the strong external coupling limit, the state is also disentangled. While there is no long-range order in  $\hat{s}_{iz}$ , there is long-range order in  $\hat{s}_{ix}$ , though it is due to the external coupling. With both coupling and interaction nonzero, any eigenstate of this Hamiltonian is always entangled [7]. Roughly speaking, entanglement at zero temperature, as an alternative to thermal fluctuation, provides the nonvanishing connected correlation function, as detailed in the next section. Some behavior of entanglement was recently investigated in a one-dimensional model [9, 10].

In low dimensional antiferromagnets, spin liquid states, e.g. the RVB state, become important. This may be understood as due to the diminishing of the effect of SSB or disentanglement. They are indeed entangled states. The amount of entanglement for a short-range RVB state on a square lattice [18] has been calculated [7]. On the other hand, it has been known that the staggered correlation function in this state is exponentially bounded [19]. This is a converse example of our argument concerning the relation between long-range order and disentanglement.

In a pure quantum state, the fluctuation amplitude is nonzero if and only if the state is not an eigenstate of the operator, i.e. the state is a superposition of its eigenstates. So if the operator involves more than one particle, e.g. if  $\hat{O} = \sum_i \hat{s}_{iz}$ , there may be entanglement. This can be seen from  $\langle \hat{O}^2 \rangle - \langle \hat{O} \rangle^2 = \sum_i (\langle \hat{s}_{iz}^2 \rangle - \langle \hat{s}_{iz} \rangle^2) + \sum_{i \neq j} \langle \hat{s}_{iz} \hat{s}_{jz} \rangle_c$ . It will be shown below that a nonzero connected correlation function  $\langle \hat{s}_{iz} \hat{s}_{jz} \rangle_c$  can characterize the entanglement between any two parts with  $i$  and  $j$  belonging to them respectively. Therefore *the quantum fluctuation of a sum of local operators is the sum of the quantum fluctuations of individual local operators and all the two-body entanglements.*

At a finite temperature, presumably the fluctuation contains both thermal and quantum ones. However, if the Hamiltonian is compatible with the operator in question, then the fluctuation is solely thermal. Moreover, although in general a connected correlation function is contributed by both thermal fluctuations and quantum entanglement, with disentanglement, it is only due to thermal fluctuation. Thermodynamic entropy only measures the population of Hamiltonian eigenstates, therefore thermal phase transitions, determined by

the competition between entropy and energetics and associated with the change of order and symmetry, is essentially classical (although the average entanglement may change with the temperature simply because different Hamiltonian eigenstates may contain different amounts of entanglement).

## 7. Connected correlation functions as characterizations of entanglements in a pure state

In this section, we discuss how the connected correlation functions can be used in characterizing entanglement. This approach has the advantage that it is not necessary to explicitly know the many-body state, and thus quite suits many-body systems. It is naturally connected with the traditional many-body techniques, and can be used to study, for example, the pairwise entanglement as a function of the distance.

For a pure state  $|\psi\rangle$ , the connected correlation function of two operators, for two bodies  $i$  and  $j$  respectively,  $\langle\hat{O}_i\hat{O}_j\rangle_c \equiv \langle\hat{O}_i\hat{O}_j\rangle - \langle\hat{O}_i\rangle\langle\hat{O}_j\rangle$ , vanishes if  $|\psi\rangle$  is any direct product of two factors to which  $i$  and  $j$  belong respectively [20].

Therefore if for certain operators  $\hat{O}_i$  and  $\hat{O}_j$ ,  $\langle\hat{O}_i\hat{O}_j\rangle_c \neq 0$ , then there is not any bipartition of the system, with  $i$  and  $j$  belonging to the two different parts, such that  $|\psi\rangle$  is a direct product of the pure states of the two parts, i.e. any part of the system with  $i$  included is entangled with its complementary part with  $j$  included.

In general, the connected correlation function of the operators of  $n$  bodies is the correlation function of these  $n$  operators deducted by all kinds of products of the connected correlation functions of proper subsets of these  $n$  operators. It measures the part of the correlation which is not due to the correlations of not all of the bodies. For example,

$$\begin{aligned}\langle\hat{O}_i\hat{O}_j\hat{O}_k\rangle_c &\equiv \langle\hat{O}_i\hat{O}_j\hat{O}_k\rangle - \\ &\quad (\langle\hat{O}_i\rangle\langle\hat{O}_j\rangle\langle\hat{O}_k\rangle + \\ &\quad \langle\hat{O}_i\hat{O}_j\rangle_c\langle\hat{O}_k\rangle + \langle\hat{O}_i\hat{O}_k\rangle_c\langle\hat{O}_j\rangle + \langle\hat{O}_j\hat{O}_k\rangle_c\langle\hat{O}_i\rangle),\end{aligned}\tag{8}$$

$$\begin{aligned}\langle\hat{O}_i\hat{O}_j\hat{O}_k\hat{O}_l\rangle_c &\equiv \langle\hat{O}_i\hat{O}_j\hat{O}_k\hat{O}_l\rangle - \\ &\quad (\langle\hat{O}_i\rangle\langle\hat{O}_j\rangle\langle\hat{O}_k\rangle\langle\hat{O}_l\rangle \\ &\quad + \langle\hat{O}_i\hat{O}_j\rangle_c\langle\hat{O}_k\rangle\langle\hat{O}_l\rangle + \cdots (6 \text{ terms}) \\ &\quad + \langle\hat{O}_i\hat{O}_j\rangle_c\langle\hat{O}_k\hat{O}_l\rangle_c + \cdots (3 \text{ terms}) \\ &\quad + \langle\hat{O}_i\hat{O}_j\hat{O}_k\rangle_c\langle\hat{O}_l\rangle + \cdots (4 \text{ terms})),\end{aligned}\tag{9}$$

and so on.

It can be seen that if  $|\psi\rangle$  contains a separable factor of a subset of  $m$  parts, and suppose  $i_1, i_2, \dots, i_m$  are  $m$  bodies belonging to these  $m$  parts respectively, then any connected correlation function of these  $m$  bodies vanishes. Of course, similar is for any connected correlation function of a subset of these  $m$  bodies. For example, suppose  $|\psi\rangle = |\phi(ij\dots)\rangle \otimes |\phi(k\dots)\rangle$ , where  $\dots$  denotes the bodies other than  $i, j, k$  if there are other bodies in the system. Then  $\langle\hat{O}_i\hat{O}_k\rangle_c = \langle\hat{O}_j\hat{O}_k\rangle_c = 0$ . Whether  $\langle\hat{O}_i\hat{O}_j\rangle_c$  vanishes depends on whether  $i$  and  $j$  can further be separated. In either case, it is certain that  $\langle\hat{O}_i\hat{O}_j\hat{O}_k\rangle_c = 0$ . If  $|\psi\rangle = |\phi(i\dots)\rangle \otimes |\phi(j\dots)\rangle \otimes |\phi(k\dots)\rangle$ , then  $\langle\hat{O}_i\hat{O}_k\rangle_c = \langle\hat{O}_j\hat{O}_k\rangle_c = \langle\hat{O}_i\hat{O}_j\rangle_c = \langle\hat{O}_i\hat{O}_j\hat{O}_k\rangle_c = 0$ .

Therefore if for certain operators  $\hat{O}_{i_1}, \dots, \hat{O}_{i_m}$ ,  $\langle\hat{O}_{i_1}\dots\hat{O}_{i_m}\rangle_c \neq 0$ , then for any  $m$ -partite partition of the system, with  $i_1, \dots, i_m$  belonging to the different  $m$  parts,  $|\psi\rangle$  does not



contain any separable factor of any proper subset of the  $m$  parts. That is to say, there exists *true  $m$ -partite entanglement* among these  $m$  parts, i.e. the entanglement cannot be reduced to the entanglement among a proper subset of the  $m$  parts. Thus a non-vanishing  $m$ -body connected correlation function characterizes the true  $m$ -partite entanglement. For example, if  $\langle \hat{O}_i \hat{O}_j \hat{O}_k \rangle_c \neq 0$ , then  $|\psi\rangle$  cannot be separated as  $|\phi(i \cdots)\rangle \otimes |\phi(j \cdots)\rangle \otimes |\phi(k \cdots)\rangle$  or  $|\phi(ij \cdots)\rangle \otimes |\phi(k \cdots)\rangle$  or  $|\phi(ik \cdots)\rangle \otimes |\phi(j \cdots)\rangle$  or  $|\phi(jk \cdots)\rangle \otimes |\phi(i \cdots)\rangle$ .

Now we consider the examples of disentanglement studied in the previous sections. The ferromagnetic or antiferromagnetic Néel state is completely separable, i.e. it is a product of the pure spin states of all the spins, hence any connected correlation of any set of spins vanishes. For ODLRO, the above discussion implies that at zero temperature, the occupation number of condensate mode is separated from the rest of the system, therefore any connected correlation function of the occupation numbers of any number of modes with one of which being the condensate mode must vanish.

What about the converse, i.e. when does the vanishing of a connected correlation imply separability? In the following, we only consider the simplest case: a two-spin state. Without loss of essence, by considering Schmidt decomposition, the state can be written as

$$|\psi\rangle = \cos\theta|\alpha_i\rangle|\gamma_j\rangle + \sin\theta|\beta_i\rangle|\delta_j\rangle, \quad (10)$$

where  $|\alpha_i\rangle$  and  $|\beta_i\rangle$ , as eigenfunctions of the spin operator  $\hat{s}_{\mathbf{n}_i}$  in a certain direction, comprise a spin basis of  $i$ , while  $|\gamma_j\rangle$  and  $|\delta_j\rangle$ , as eigenfunctions of a certain  $\hat{s}_{\mathbf{n}_j}$ , comprise a spin basis of  $j$ . The basis states for the two-spin system can be chosen to be  $|\chi_1\rangle = |\psi\rangle$ ,  $|\chi_2\rangle = -\sin\theta|\alpha_i\rangle|\gamma_j\rangle + \cos\theta|\beta_i\rangle|\delta_j\rangle$ ,  $|\chi_3\rangle = |\alpha_i\rangle|\delta_j\rangle$  and  $|\chi_4\rangle = |\beta_i\rangle|\gamma_j\rangle$ . Then  $\langle \hat{s}_{\mathbf{n}_i} \hat{s}_{\mathbf{n}_j} \rangle_c = \langle \psi | \hat{s}_{\mathbf{n}_i} \hat{P}^\perp \hat{s}_{\mathbf{n}_j} | \psi \rangle$ , where  $\hat{P}^\perp \equiv 1 - |\psi\rangle\langle\psi| = |\chi_2\rangle\langle\chi_2| + |\chi_3\rangle\langle\chi_3| + |\chi_4\rangle\langle\chi_4|$  is the projection onto the subspace orthogonal to  $|\psi\rangle$ . With eigenvalues of each spin operator being  $\pm 1/2$ , one obtains  $|\langle \hat{s}_{\mathbf{n}_i} \hat{s}_{\mathbf{n}_j} \rangle_c| = \sin^2\theta \cos^2\theta$ .

Therefore if  $\langle \hat{s}_{\mathbf{n}_i} \hat{s}_{\mathbf{n}_j} \rangle_c = 0$ , then  $|\psi\rangle$  is a direct product of pure states of  $i$  and  $j$ . To use this result, one first needs to find  $\hat{s}_{\mathbf{n}_i}$  and  $\hat{s}_{\mathbf{n}_j}$  by, say, diagonalizing the reduced density matrices of each spin.

Finally we mention that all the connected correlation functions of operators  $\hat{O}_1, \hat{O}_2, \dots$  can be obtained from a generating functional  $F\{\mathbf{h}\} \equiv \ln Z\{\mathbf{h}\}$ , with  $Z\{\mathbf{h}\} = \langle e^{\mathbf{h} \cdot \hat{\mathbf{O}}} \rangle$ ,  $\mathbf{h} \equiv (h_1, h_2, \dots)$ ,  $\hat{\mathbf{O}} \equiv (\hat{O}_1, \hat{O}_2, \dots)$ , where the subscripts denote the different bodies in the system. The connected correlation functions of  $\hat{O}_{i_1}, \dots, \hat{O}_{i_n}$  can be obtained as

$$\langle O_{i_1} \cdots \hat{O}_{i_n} \rangle_c = \frac{\delta^n F}{\delta h_{i_1} \cdots \delta h_{i_n}} \Big|_{\mathbf{h}=0}. \quad (11)$$

## 8. Summary

We have shown that off-diagonal long-range order leads to disentanglement between the condensate mode and the rest of the system. Furthermore, it is revealed that in general, diminishing of entanglement underlies various long-range orders and spontaneous symmetry breaking. This is consistent with the wisdom that Landau theory of order and symmetry breaking is essentially classical, even though the order parameter has a quantum origin [21]. Remarks are also made on the relations between entanglement on one hand, and fluctuation and correlation functions on the other. Entanglements in a pure state can be characterized in terms of the nonvanishing connected correlation functions.

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  - [1] P. W. Anderson, *Basic Notions of Condensed Matter Physics* (Benjamin, London, 1983).
  - [2] C. N. Yang, *Rev. Mod. Phys.* **34**, 694 (1962).
  - [3] W. Kohn and D. Sherrington, *Rev. Mod. Phys.* **42**, 1 (1970).
  - [4] E. Einstein, B. Podolsky and N. Rosen, *Phys. Rev.* **47**, 777 (1935); E. Schrödinger, *Proc. Camb. Phi. Soc.* **31**, 555 (1935);
  - [5] J. S. Bell, *Physics* **1**, 195 (1964).
  - [6] Y. Shi, *Ann. Phys.* **9**, 637 (2000).
  - [7] Y. Shi, quant-ph/0204058.
  - [8] Y. Shi, quant-ph/0205069.
  - [9] A. Osterloh, L. Amico, G. Falci, R. Fazio, *Nature*, **416**, 608 (2002).
  - [10] T. J. Osborn and M. A. Nielsen, *Phys. Rev. A* **65**, 042323 (2002).
  - [11] C. H. Bennett, H. J. Bernstein, S. Popescu and B. Schumacher, *Phys. Rev. A* **53**, 2046 (1996).
  - [12] W.K. Wootters, *Phys. Rev. Lett.* **80**, 2245 (1996).
  - [13] A. J. Leggett, *Rev. Mod. Phys.* **73**, 307 (2001).
  - [14] R. Peierls, *J. Phys. A* **24**, 5273 (1991).
  - [15] D. Giulini *et al.*, *Decoherence and the Appearance of a Classical World in Quantum Theory* (Springer, Berlin, 1996).
  - [16] A. J. Leggett, in A. Griffin, D. W. Snoke and S. Stringari (ed.), *Bose-Einstein Condensation* (Cambridge University, Cambridge, 1995).
  - [17] W. H. Zurek, S. Habib and J. P. Paz, *Phys. Rev. Lett.* **70**, 1187 (1993).
  - [18] S. A. Kivelson, D. S. Rokhsar and J. P. Sethna, *Phys. Rev. B* **35**, 8865 (1987).
  - [19] M. Kohmoto and Y. Shapir, *Phys. Rev. B* **37**, 9439 (1987).
  - [20] The special case that a two-body connected correlation function vanishes for a product state was also noted in Ref. [10] (under the term “spin-spin correlation function”).
  - [21] Recently a so-called quantum order was studied which cannot be described in terms of Landau theory and in which entanglement may be important [X. G. Wen, *Phys. Lett. A* **300**, 175 (2002)].